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Energy levels, oscillator strengths and lifetimes in Mg-like sulphur

G P Gupta and A Z Msezane*

Department of Physics, S D (Postgraduate) College, University of Meerut, Muzaffarnagar-251 001, India

*Department of Physics and CTSPS, Clark Atlanta University, Atlanta, Georgia 30314, USA

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Abstract Energy levels between the ground and the various excited states, oscillator strengths and transition probabilities for all dipole-allowed transitions among the 24 LS target states $3s^2(^1S)$, $3s3p(^{1,3}P^0)$, $3p^2(^1S,^3P,^1D)$, $3s3d(^{1,3}D)$, $3s4s(^{1,3}S)$, $3p3d(^{1,3}P^0, ^{1,3}D^0, ^{1,3}F^0)$, $3s4p(^{1,3}P^0)$, $3s4d(^{1,3}D)$, $3s4f(^{1,3}F^0)$ and $3p4s(^{1,3}P^0)$ of S *V* are calculated using program CIV3 of Hibbert. Extensive configuration-interaction target wave functions are used in the calculation. From our transition probabilities, we have also evaluated radiative lifetimes of singlet and triplet states in S *V*. Our calculated energy values, oscillator strengths and lifetimes are compared with the experimental and other theoretical results

Keywords Atomic data, energy levels, wave functions

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1. Introduction

Emission lines due to S *V* ions have been detected in the ultraviolet (UV) spectra from the Io plasma torus in the magnetosphere of Jupiter during the Voyager I encounter [1,2]. Spectral lines due to allowed and semi-forbidden transitions between levels in S *V* have also been observed in the UV and X-ray regions of the solar spectrum [3]. The emission lines in the wavelengths region from 1100–2000 Å in the solar spectrum are recorded by the NRL normal-incidence slit spectrograph (S082-B) on Skylab [4–6]. Joelsson *et al* [7] have observed the spectra from sliding spark and beam-foil sources over the 187–6729 Å region and classified some 385 lines as S *V* transitions. Accurate atomic data such as absorption oscillator strengths and transition probabilities in S *V* are useful in many astrophysical studies and are also needed for solar and stellar abundance calculations [8].

Most of the experimental and theoretical data available in the literature are limited to allowed transitions involving the few lowest states in LS coupling scheme. The experimental oscillator strengths and lifetimes in S *V* have been measured by several workers [9–11] using beam-foil techniques. Theoretically, Crossley and Dalgarno [12] reported the oscillator strengths and lifetimes for few dipole-allowed transitions in S *V*. Victor *et al* [13] performed a configuration-interaction (CI) calculation of oscillator strengths in the Mg isoelectronic sequence, within a semiempirical model potential framework. Van Wyngaarden and Henry [14] used CI target wave functions and reported the oscillator strengths and collision strengths for the first four UV lines.

Recently, Gupta and Msezane [15] calculated energy levels, oscillator strengths, and transition probabilities for all dipole-allowed transitions among the 25 low lying levels of S *IV* in LS coupling scheme using the CIV3 computer code of Hibbert [16]. In this work, we have extended our calculation of these parameters for all dipole-allowed transitions among the 24 terms belonging to $(1s^22s^22p^6)3s^2$, $3s3p$, $3s3d$, $3p^2$, $3p3d$, $3s4s$, $3s4p$, $3s4d$, $3s4f$ and $3p4s$ configurations of S *V*. We included a fairly large number of configurations within the $n = 5$ complex in the CI expansion. The radiative lifetimes of singlet and triplet states in S *V* are also calculated from our radiative decay rates.

2. Choice of wave functions

The ionic state wave functions of each of the 24 LS target states $3s^2(^1S)$, $3s3p(^{1,3}P^0)$, $3p^2(^1S,^3P,^1D)$, $3s3d(^{1,3}D)$, $3s4s(^{1,3}S)$, $3p3d(^{1,3}P^0, ^{1,3}D^0, ^{1,3}F^0)$, $3s4p(^{1,3}P^0)$, $3s4d(^{1,3}D)$, $3s4f(^{1,3}F^0)$ and $3p4s(^{1,3}P^0)$ of S V are written in terms of CI expansions

$$\psi(LS\pi) = \sum_{i=1}^{M} a_i \phi_i(\alpha_i LS\pi), \qquad (1)$$

where each single-configuration function ϕ_i is constructed from one-electron orbitals whose angular momenta are coupled to give total L, S and π. M is the number of configurations and α_i specifies the angular momentum coupling scheme of the i-th configuration. The radial parts of the one-electron functions are expressed in analytic form as a sum of Slater-type orbitals

$$P_{nl} = \sum_{i=1}^{k} C_i \left[(2\zeta_i)^{p_i+1} / (2p_i)! \right]^{1/2} r^{p_i} \exp(-\zeta_i r) \quad (2)$$

The parameters C_i, ζ_i and p_i in equation (2) are determined variationally as described by Hibbert [16].

In our calculation we used the 15 orthogonal one-electron orbitals 1*s*, 2*s*, 2*p*, 3*s*, 3*p*, 3*d*, 4*s*, 4*p*, 4*d*, 4*f*, 5*s*, 5*p*, 5*d*, 5*f* and 5*g* out of which the first four radial functions are taken as the Hartree-Fock orbitals of the ground state $(1s^2 2s^2 2p^6)3s^2$ (^1S) of S I given by Clementi and Roetti [17]. The 3*p*, 3*d*, 4*s*, 4*p*, 4*d* and 4*f* functions are chosen as spectroscopic-type orbitals and are optimized on the excited states $3s3p(^3P^0)$, $3s3d(^3D)$, $3s4s(^3S)$, $3s4p(^3P^0)$, $3s4d(^3D)$ and $3s4f(^3F^0)$, respectively. In order to represent all the energy levels by a single set of orthogonal functions, we have chosen the 5*s*, 5*p*, 5*d*, 5*f* and 5*g* orbitals as correlation-type orbitals and optimized them on the $3d4d(^1D)$, $3p3d(^3D^0)$, $3p3d(^1F^0)$, $3p3d(^3D^0)$ and $3s3d(^1F^0)$ states, respectively. In all cases we chose $k = n - 1$ so that the coefficients C_i and uniquely specified by the orthogonality condition on P_{nl}. The parameters of the optimized radial functions are displayed in Table 1. The convergence of CI expansions is tested up to two-electron excitation from the basic configurations used in this calculation. We considered configurations within the $n = 5$ complex in the CI expansion to ensure convergence. These CI wave functions are used to calculate energy levels, oscillator strengths, and radiative transition probabilities.

The radiative lifetime of an excited state is calculated from radiative transition probabilities A_{ji} using the relation

$$\tau_j = 1/\Sigma_i A_{ji} \quad (3)$$

where the sum over i is over all accessible final states.

Table 1. Radial function parameters for optimized orbitals of S I

Orbitals	C_i	p_i	ζ_i
3*p*	0.3405240	2	6.1701774
	1.0329943	3	2.2288851
3*d*	1.0000000	3	2.0147914
4*s*	0.0755291	1	12.8393616
	0.3082528	2	5.1837950
	1.0728670	3	2.3379781
	1.4559718	4	1.6482533
4*p*	0.1916326	2	6.2964445
	1.4819812	3	1.7691246
	1.9584639	4	1.5613560
4*d*	0.6353479	3	2.1594933
	1.1474627	4	1.1969040
4*f*	1.0000000	4	1.2780449
5*s*	0.2461588	1	12.6729509
	3.0638317	2	3.4256202
	5.3679309	3	3.1810846
	1.2797951	1	2.5618566
	2.1116791	5	2.1181415
5*p*	7.6018305	2	2.3510508
	34.7834270	3	2.3037243
	93.0085011	4	2.1013755
	67.9356379	5	2.3459375
5*d*	0.9598501	3	5.2327287
	12.8032778	4	1.4900826
	12.8001661	5	1.8112120
5*f*	1.3172764	4	2.2578557
	0.9221017	5	1.5391259
5*g*	1.0000000	5	2.6469708

3. Results and discussion

3.1 Energy levels

In Table 2, we present our *ab initio* energies of the 24 low-lying levels relative to the ground level. These are compared with the experimental results of Joelsson *et al* [7] compiled by Martin *et al* [18]. The experimental results of Moore [19]

Table 2. Calculated and experimental energy levels (in a.u.) of S I

Index	Level		Present	Experiment		Other theory	
				MZM	MR	WH	DK
1	$3s^2$	^1S	0.0000	0.0000	0.0000	0.0000	0.0000
2	$3s3p$	$^3P^0$	0.3741	0.3817	0.3819	0.3696	0.3759
3		$^1P^0$	0.5836	0.5793	0.5794	0.5847	0.5847
4	$3p^2$	^1D	0.8734	0.8827	0.8772	0.8652	0.8759
5		^3P	0.9091	0.9147	0.9150	0.9015	0.9133
6	$3s3d$	^1D	1.0622	1.0705	1.0708	1.0675	1.0789
7	$3p^2$	^1S	1.0744	1.0723			1.0781
8	$3s3d$	^1D	1.2348	1.2334			1.2816
9	$3s4s$	^3S	1.4090	1.4197	1.4202	1.4166	
10		^1S	1.4517	1.4585			
11	$3p3d$	$^1F^0$	1.4591	1.4748			
12		$^1D^0$	1.4834	1.4965			
13		$^1P^0$	1.5639	1.5744			
14		$^3D^0$	1.5765	1.5858			
15	$3s4p$	$^3P^0$	1.5795	1.5917			
16		$^1P^0$	1.5811	1.5926			
17	$3p3d$	$^1F^0$	1.6635	1.6715			
18		$^1P^0$	1.7263				
19	$3s4d$	^3D	1.7920	1.8045			
20		^1D	1.7998	1.8116			
21	$3s4f$	$^3F^0$	1.8575	1.8723			
22		$^1F^0$	1.8952	1.9045			
23	$3p4s$	$^3P^0$	1.9081	1.9206			
24		$^1P^0$	1.9386	1.9343			

MZM Experimental results of Joelsson *et al* [7] compiled by Martin *et al* [18]. MR Moore [19]. WH Wyngaarden and Henry [14]. DK Dutton and Kingston [20]

and the calculated energies of Van Wyngaarden and Henry [14] and Dufton and Kingston [20] are also presented for comparison. It is seen from the table that the two experimental results are very close to each other and the ordering of our calculated excitation energies is the same as that of the experimental data. Our energy values agree to better than 1% with the measured values, except for the $3s3p(^3P^0)$ state where the difference between our calculated value and the experimental result is 2%. For this level, the result of Dufton and Kingston [20] agrees with our calculation while the calculation of Van Wyngaarden and Henry [14] differ significantly with the other theoretical and experimental results. For other levels, the calculations of Van Wyngaarden and Henry [14] and Dufton and Kingston [20] agree reasonably well with the other results. It may be worth mentioning that we found a strong mixing between the $3s3d(^1D)$ and $3p^2(^1D)$ as well as the $3s4f(^1F^0)$ and $3p3d(^1F^0)$ states.

Table 3. Transition probabilities and oscillator strengths for allowed transitions in S *V*

Transitions from lower to upper level	Present calculation			Experiment	Other calculations[*]	
	A_l	f_l	f_v		f_L	f_v
$3s^2(^1S) - 3s3p(^1P^0)$	5.2607 + 09	1.4422	1.4634	1.06 ± 0 08[a]	1 4380	1.399[m]
				1 41 ± 0 10[b]	1.360	
					1 460[n]	
$3s4p(^1P^0)$	2 3916 + 09	0.0893	0 0880		0 1370	
$3p3d(^1P^0)$	9.0820 + 07	0 0028	0.0022		0.0014	
$3p4s(^1P^0)$	3.4294 + 06	0.0001	0.0000		0.0091	
$3s3p(^1P^0) - 3p^2(^1D)$	1.6285 + 08	0.1020	0 0993		0.1020	
$3p^2(^1S)$	4 3290 + 09	0 1864	0 2040		0 1800	
$3s3d(^1D)$	1.1783 + 10	1.4413	1.4925	0 91 ± 0 14[a]	1.3360	1.285[m]
				1 24 ± 0.14[c]	1 380	
$3s4s(^1S)$	6 1843 + 09	0 0851	0 0808		0.0725	
$3s4d(^1D)$	2 8071 + 08	0.0098	0 0036		0.0043	
$3p^2(^1D) - 3p3d(^1D^0)$	5.1379 + 09	0 4270	0.4551		0.3990	
$3s4p(^1P^0)$	1.7639 + 09	0.0654	0 0706		0 0674	
$3p3d(^1F^0)$	9,7766 + 09	0 6790	0 6996			
$3p3d(^1P^0)$	2.5606 + 06	0.0001	0.0000		0.0000	
$3s4f(^1F^0)$	3 9668 + 08	0.0165	0 0173			
$3p4s(^1P^0)$	6.8521 + 09	0.1124	0 1086		0 1130	
$3p^2(^1S) - 3s4p(^1P^0)$	1 4343 + 08	0 0522	0 0572		0 0610	
$3p3d(^1P^0)$	7.1291 + 09	1.5662	1 6524		1 5300	
$3p4s(^1P^0)$	1.3608 + 09	0 1701	0.1829		0.1300	
$3s3d(^1D) - 3p3d(^1D^0)$	6.2341 + 07	0 0314	0.0295		0 0304	
$3s4p(^1P^0)$	6.6185 + 08	0 1031	0.1041		0.0998	
$3p3d(^1F^0)$	1.4714 + 09	0.3489	0.3791			
$3p3d(^1P^0)$	1.8517 + 09	0 1431	0.1566		0 1420	
$3s4f(^1F^0)$	1.2349 + 10	1.2338	1.2386			
$3p4s(^1P^0)$	1.9227 + 09	0.0725	0.0716		0.0465	
$3s4s(^1S) - 3s4p(^1P^0)$	1 0892 + 08	0.6068	0.6820		0.6610	
$3p3d(^1P^0)$	3.4344 + 07	0.0425	0.0530		0.0354	
$3p4s(^1P^0)$	2.6086 + 09	1.0273	1.0512		1.0900	
$3p3d(^1D^0) - 3s4d(^1D)$	1.1347 + 06	0.0004	0 0008		0.0005	
$3s4p(^1P^0) - 3s4d(^1D)$	7.9608 + 08	0 8638	0 8361		0.8690	
$3p3d(^1F^0) - 3s4d(^1D)$	4.4035 + 07	0.0527	0.0536			
$3p3d(^1P^0) - 3s4d(^1D)$	8.5894 + 05	0.0083	0.0199		0.0069	

Table 3. *(Cont'd)*

Transitions from lower to upper level	Present calculation			Experiment	Other calculations+	
	A_L	f_l	f_v		f_l	f_v
$3s4d(^1D)$ - $3s4f(^1F^0)$	6.6138 + 07	0.3164	0.3388			
$3s4d(^1D)$ – $3p4s(^1P^0)$	3 4953 + 05	0 0003	0 0152		0.0164	
$3s3p(^3P^0)$ - $3p^2(^3P)$	4 4746 + 09	0.4866	0 5043	0 35 ± 0.02[a]	0 492	0.484[m]
				0 15 ± 0.20[b]	0.460[n]	
$3s3d(^3D)$	6 6539 + 09	0.7289	0.7671	0.64 ± 0.06[d]	0.741	0.710[m]
				0.55 ± 0.02[c]	0.68	
					0.700[n]	
$3s4s(^1S)$	1 0532 + 10	0.1020	0 1031		0.103	0.098[m]
					0.0987	
$3s4d(^1D)$	1 1625 + 09	0.0300	0.0270		0.0355	
$3p^2(^1P)$ $3p3d(^1P^0)$	5 2913 + 09	0 3841	0 4142		0.3560	
$3p3d(^1D^0)$	9.4067 + 09	1 0955	1 1688		1.0300	
$3s4p(^1P^0)$	1 1259 + 07	0 0008	0 0006		0.0065	
$3p4s(^1P^0)$	6 1289 + 09	0 1911	0 1905		0 1770	
$3s3d(^1D)$ - $3p3d(^1F^0)$	7 0776 + 08	0 1958	0.1982			
$3p3d(^1P^0)$	2 4004 + 09	0 1781	0 1863		0 1880	
$3p3d(^1D^0)$	2 0854 + 09	0 2454	0 2569		0.2310	
$3s4p(^1P^0)$	1 2936 + 09	0 0903	0.0937		0.0788	
$3s4f(^1F^0)$	1 2868 + 10	0 8867	0.8968			
$3p4s(^1P^0)$	5 2343 + 07	0 0014	0 0018		0 0013	
$3s4s(^1S)$ – $3p3d(^1P^0)$	1 1863 + 06	0 0046	0 0029		0.0175	
$3s4p(^1P^0)$	3 0447 + 08	0 9778	0 9946		0.9890	
$3p4s(^3P^0)$	2 1406 + 09	0 8022	0 8548		0 7560	
$3p3d(^3F^0)$ - $3s4d(^1D)$	6 5368 + 07	0 0131	0 0115			
$3p3d(^1P^0)$ – $3s4d(^3D)$	5 6930 + 06	0 0057	0 0049		0 0181	
$3p3d(^1D^0)$ $3s4d(^1D)$	1 4567 + 05	0 0001	0 0001		0 0011	
$3s4p(^3P^0)$ - $3s4d(^1D)$	7 9767 + 08	0 9160	0 8791		0.8800	
$3s4d(^1D)$ - $3s4f(^1F^0)$	2 4345 + 07	0 2474	0 2156			
$3s4d(^1D)$ – $3p4s(^3P^0)$	5 1670 + 05	0 0007	0 0032		0.0002	

a Irwin and Livingston [10], b Berry *et al* [9], c Dumont *et al* [11], m . Wyngaarden and Henry [14], n Crossley and Dalgarno [12], + Victor *et al* [13]

3.2 Oscillator strengths and radiative decay rates :

In Table 3, we have listed our radiative decay rates in the length form A_l and the absorption oscillator strengths in both length f_l and velocity f_v formulations for all dipole-allowed transitions among the 24 LS levels. A very good agreement between the length and velocity values of the oscillator strengths for most transitions, to some extent, indicates the high quality of our wave functions used in calculating these parameters. The experimental results are available for only a few transitions and there are considerable differences among the experimental data for these transitions. For the transitions $3s^2(^1S)$–$3s3p(^1p^0)$ and $3s3p(^1P^0)$–$3s3d(^1D)$ our calculated values are closer to the experimental results of Berry *et al* [9] and Dumont *et al* [11], while for the $3s3p(^3P^0)$–$3p^2(^3P)$ and $3s3p(^3P^0)$–$3s3d(^3D)$ our values are closer to the experimental results of Irwin and Livingston [10]. Our results for these four transitions are in good agreement with the other theoretical calculations. For the rest of the transitions, our results are compared with the theoretical values of Victor *et al* [13]. The two calculations agree well

for almost all the strong transitions, but differ significantly for a few weaker transitions.

3 3. Lifetimes :

In Table 4, we present our calculated radiative lifetimes [using equation (3)] for singlet and triplet states. These are compared with the experimental results of Dumont *et al* [11] and Irwin and Livingston [10] and the other theoretical calculations of Crossley and Dalgarno [12] and Victor *et al* [13]. Lifetimes for the $3p3d(^1D^0)$, $3p3d(^3P^0)$, $3p3d(^3D^0)$ and $3s4p(^3P^0)$ states are also calculated to make these compatible with the experimental results. From the table it is seen that our calculated values are in good agreement with the experimental results, except for the $3s3p(^1P^0)$, $3p3d(^1D^0)$ and $3p^2(^3P)$ states where our results are within 30%, 25% and 26% respectively, with the experimental data. Further, for the $3p^2(^3P)$–$3p3d(^3P^0)$ transition our calculated lifetime agrees reasonably well with both the experimental results while for the $3s3p(^3D)$–$3p3d(^3P^0)$ the difference is a factor of 2 between our data and those of Irwin and Livingston [10]. Our calculated values agree very well with the theoretical results of Crossley and Dalgarno [12] and Victor *et al* [13], except for the $3p3d(^3F^0)$ state where our result agrees well with the experiment but differs with the calculation of Crossley and Dalgarno [12].

4. Conclusion

In conclusion, we have presented an extensive CI calculation of energy levels between the ground state and the various excited states as well as oscillator strengths and transition

Table 4. Lifetimes (in nanoseconds) of singlet and triplet states in S I.

Upper state	Present+	Experiment		Other theory	
		DGB	IL	CD	VSL
$3s3p(^1P^0)$	0.1901	0.280 ± 0.01	0.263 ± 0 018	0.200	0.200
$3p^2(^1D)$	6.1406				
$3p^2(^1S)$	0.2310				
$3s3d(^1D)$	0.0849	0.098 ± 0 01	0 130 ± 0.020	0 105	0.088
$3s4s(^1S)$	0 1617				
$3p3d(^1D^0)$	0 1923			0.230	0.210
	0 1946*1	0.270 ± 0 01			
$3s4p(^1P^0)$	0.1973				
$3p3d(^1F^0)$	0 0889				
$3p3d(^1P^0)$	0.1098				
$3s4d(^1D)$	0.8906				
$3s4f(^1F^0)$	0 0781				
$3p4s(^1P^0)$	0 0784				
$3p^2(^1P)$	0.2235	0.280 ± 0.03	0 320 ± 0.020	0 240	0.240
$3s3d(^1D)$	0 1503	0.200 ± 0 008	0 172 ± 0.014	0 150	0 160
$3s4s(^3S)$	0.0995				
$3p3d(^3F^0)$	1 4129	1 2 ± 0 2		1.000	
$3p3d(^3P^0)$	0 1300			0 140	0.130
	0.1890*2	0 14 ± 0 02	0 200 ± 0.030		
	0 4166*1		0 260 ± 0.040		
$3p3d(^3D^0)$	0 0870			0 090	0.090
	0.1063*4	0.10 ± 0 01			
$3s4p(^1P^0)$	0.6214			0.640	0.640
	0.7730*5	0 79 ± 0.05			
$3s4d(^3D)$	0.4923				
$3s4f(^3F^0)$	0 0776				
$3p4s(^3P^0)$	0 1202				

DGB : Dumont *et al* [11], IL . Irwin and Livingston [10], CD : Crossley and Dalgarno [12], VSL · Victor *et al* [13], + . Results calculated using equation (3), *1 : Results for transition $3p^2(^1D)$ - $3p3d(^1D^0)$, *2 : Results for transition $3p^2(^3P)$ - $3p3d(^3P^0)$, *3 · Results for transition $3s3d(^3D)$ - $3p3d(^3P^0)$, *4 : Results for transition $3p^2(^3P)$ - $3p3d(^3D^0)$, *5 . Results for transition $3s3d(^3D)$ - $3s4p(^3P^0)$.

probabilities for all dipole-allowed transitions among the 24 terms arising from the terms belonging to the $(1s^2 2s^2 2p^6)3s^2$, $3s3p$, $3s3d$, $3p^2$, $3p3d$, $3s4s$, $3s4p$, $3s4d$, $3s4f$ and $3p4s$ configurations of S *V*. Program CIV3 of Hibbert [16] has been used for the calculation. As seen in Table 2, our *ab nitio* energies are in excellent agreement with the recent measurement of Joelsson *et al* [7] for all the excited states. Also a very good agreement between the length and velocity values of our oscillator strengths for most transitions is indicative of the overall accuracy of wave functions used in this calculation. Generally, our results agree reasonably well with those from the experiments and the other theoretical calculations. The results presented in this work are quite extensive and include the important correlation effects in the excitation to the $5g$ orbital. We believe that our results would be useful in many astrophysical applications.

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